International Scientific Colloquium
Modelling for Material Processing
Riga, June 8-9, 2006

About the Numerical Simulation of Heat and Moisture Diffusion in Porous Media

H. Kalis, I. Kangro

Abstract

The article features the system of two partial differential equations, which describes the distribution of temperature T and moisture C in porous media depending on the physical parameters. The temperature and moisture change development (dynamics) in time during moisturising and drying processes is under examination. The methodology, developed in the current research, allows reducing the system of the partial differential equations to a single PDE of diffusion in relation to C and T.

Introduction

Let us explore the diffusion process by emitting or absorbing heat through pores of solid objects, i.e. moisture transfer and heat transfer. Adequate equations can be added up by characterising the diffusion process of two substances in porous media – one replacing the other, notwithstanding the thermal effects. When constructing numerical algorithms, it is possible to add additionally fixed source functions to the right side of the process characterising equation.
A typical example might be package fabric fibres with air spaces, where water penetrates the fibres through diffusion or moisturising and drying of a wood plate (material).

1. Mathematical Model

If we accept a linear relevance between temperature T and moisture M , a balance equation in the package under research can be written [1]: $M = const + \sigma C - \omega T$,
where C is the concentration of water vapour in air spaces, M - amount of moisture absorbed by unit mass of fibre, σ, ω - positive constants. Thus the equation governing the movement of vapour can be written [1]

$$\partial(D \partial C / \partial z) / \partial z = m \partial C / \partial t + (1-m) \rho_S \partial M / \partial t , \qquad (1.1)$$

where $z \in [0, L]$, $2L$ - thickness of layer, due to the symmetry the process is investigated only in the one half of the layer. D is the diffusion coefficient for moisture in the air, m is a fraction of the total volume of the package occupied by air, $1-m$ the total volume of the package occupied by fibre of density ρ_S (if $m = 1$ then the classic equation of diffusion is obtained).
For taking out the heat conductivity equation, it is assumed that the rate at which the temperature of the element changes is determined by conduction of heat through air and fibres and the heat evolved when fibres absorbed the moisture [1]:

$$c \rho \partial T / \partial t = \partial(K \partial C / \partial z) / \partial z + q \rho \partial M / \partial t , \qquad (1.2)$$

where c - the specific heat of the fibres, ρ - the density of the package, expressed as mass of fibre per unit overall volume, q - the heat evolved when water vapour is absorbed by the fibres, K - the overall heat conductivity of the package.
Supposing that all the coefficients are constants and eliminating M from (1.1), (1.2) one obtains the system of PDE with respect to T , C:

$$\begin{cases} D^T \partial^2 T / \partial z^2 = \partial T / \partial t - \nu \partial C / \partial t \\ D^C \partial^2 C / \partial z^2 = \partial C / \partial t - \lambda \partial T / \partial t \end{cases}, \tag{1.3}$$

where $D^T = K / (\rho (c + q\omega))$, $D^C = D / (m + (1-m)\rho_S \sigma)$ are the corresponding coefficients of diffusion and concentration of water vapour, $\nu = q\sigma / (c + q\omega)$ and $\lambda = ((1-m)\omega\rho_S) / (m + (1-m)\rho_S \sigma)$ - coefficients at the source elements $\partial C / \partial t$, $\partial T / \partial t$ in the above - mentioned equations. It is possible to reduce the system of PDE (1.3) by adding to its right side the source functions – the two given functions $f_1(z,t)$ and $f_2(z,t)$:

$$\begin{cases} D^T \partial^2 T / \partial z^2 = \partial T / \partial t - \nu \partial C / \partial t + f_1(z,t) \\ D^C \partial^2 C / \partial z^2 = \partial C / \partial t - \lambda \partial T / \partial t + f_2(z,t) \end{cases}. \tag{1.4}$$

At first let us consider for $z \in [0, L]$ the boundary conditions of the first type if $z = 0$, i.e. given T C values. If $z = L$, than due to the symmetry conditions we find $\partial T / \partial z = \partial C / \partial z = 0$.

2. Reduction of the System of PDE in Two Independent Differential Equations

Consequently [1], in the case of the boundary conditions of the first type, by multiplying the first equation of the system (1.4) with ratio s / D^T, but the second - with r / D^C (r, s - temporarily unknown constants), by adding two mentioned equations we obtain one PDE of diffusion with respect to $V = sT + rC$ in the form

$$\mu^{-1} \partial^2 V / \partial z^2 = \partial V / \partial t + s / (D^T \mu) f_1 + r / (D^C \mu) f_2, \tag{2.1}$$

where μ^{-1} is the corresponding coefficient of diffusion $(\mu > 0)$.
It is possible to obtain two independent PDE with respect to functions V_1 and V_2

$$\mu_1^{-1} \partial^2 V_1 / \partial z^2 = \partial V_1 / \partial t + g_1, \tag{2.2}$$

$$\mu_2^{-1} \partial^2 V_2 / \partial z^2 = \partial V_2 / \partial t + g_2 \tag{2.3}$$

where $V_1 = C - m_2 T$, $g_1 = s_1 f_1 / (r_1 D^T \mu_1) + (D^C \mu_1)^{-1} f_2$,
$V_2 = T - m_1 C$, $g_2 = r_2 f_2 / (r s_2 D^C \mu_2) + (D^T \mu_2)^{-1} f_1$, $m_1 = (1 - \mu_1 D^C) / \nu$, $m_2 = (1 - \mu_2 D^T) / \nu$, $\mu_1 = (d_1 + d_2 / d_3)$, $\mu_2 = (d_1 - d_2 / d_3)$, $d_1 = D^T + D^C$, $d_2 = \sqrt{(D^T - D^C)^2 + 4\lambda\nu D^T D^C}$, $d_3 = 2 D^T D^C$. If V_1, V_2 have been calculated, considering the corresponding boundary conditions and the initial conditions, t it is possible to find out, $T = \gamma^{-1}(V_2 + m_1 V_1)$, $C = \gamma^{-1}(V_1 + m_2 V_2)$, $\gamma = 1 - m_1 m_2$.

3. Analytical Solution in the Infinite Layer ($L = \propto$)

Considering the initial – boundary problem in the infinite layer –half – plane, $z \in [0, \propto]$

$$\partial V / \partial t = \mu^{-1} \partial^2 V / \partial z^2 - g(z,t),\ V\big|_{z=0} = 1,\ V\big|_{z=\propto} = 0,\ V\big|_{t=0} = 0 \qquad (3.1)$$

it is possible to obtain its solution, if $g(z,t) = 0$ in the analytical form [3, 4]:

$$V(z,t) = 1 - erf\left(z\sqrt{\mu} / \left(2\sqrt{t}\right)\right), \qquad (3.2)$$

where $erf(y) = 2/\sqrt{\pi}\int_0^y e^{-\varsigma^2} d\varsigma$ is the integral of probability $\left(erf(\propto) = 1\right)$.

Investigating the moisturising process ($C\big|_{t=0} = T\big|_{t=0} = 0$, $C\big|_{z=0} = 1, T\big|_{z=0} = 0$, and $C\big|_{z=\propto} = T\big|_{z=\propto} = 0$), we obtain $V_1\big|_{z=0} = 1$, $V_1\big|_{z=\propto} = 0$, $V_1\big|_{t=0} = 0$ and the solution corresponding the equation (3.1) is in the form $V_1(z,t) = 1 - erf\left(e_1\right)$, $e_1 = z\sqrt{\mu_1} / \left(2\sqrt{t}\right)$.

Analogically, $V_2\big|_{z=0} = -m_1$, $V_2\big|_{z=\propto} = 0$, $V_2\big|_{t=0} = 0$ and the solution is $V_2(z,t) = -m_1\left(1 - erf\left(e_2\right)\right)$, $e_2 = z\sqrt{\mu_2} / \left(2\sqrt{t}\right)$.

Thus $T(z,t) = \gamma^{-1}\left(V_2(z,t) + m_1 V_1(z,t)\right) = m_1\gamma^{-1}\left(erf(e_2) - erf(e_1)\right)$, (3.3)

$C(z,t) = \gamma^{-1}\left(V_1(z,t) + m_2 V_2(z,t)\right) = 1 + \left(\gamma^{-1} - 1\right) erf(e_2) - \gamma^{-1} erf(e_1)$.

Investigating the drying process with given external temperature ($C\big|_{t=0} = 1$, $T\big|_{t=0} = 0$, $C\big|_{z=0} = 0$, $T\big|_{z=0} = 1$ and $C\big|_{z=\propto} = 1$, $T\big|_{z=\propto} = 0$) we obtain $V_1(z,t) = -m_2 + \left(1 + m_2\right) erf\left(e_1\right)$, $V_2(z,t) = 1 - \left(m_1 + 1\right) erf\left(e_2\right)$.

Thus $T(z,t) = 1 + \left(m_1 + 1\right)\gamma^{-1}\left(erf(e_1) - erf(e_2)\right) - erf(e_1)$, (3.4)

$C(z,t) = erf(e_2) + \left(m_2 + 1\right)\gamma^{-1}\left(erf(e_1) - erf(e_2)\right)$

4. Numerical Solution in the Finite Layer by Solving Separate Equations

Solving the initial – boundary problem for the diffusion equation (3.1) in the finite layer $\left(L \neq \propto\right)$ with the boundary conditions $V\big|_{z=0} = \tilde{V}_0 = const$, $\partial V / \partial z\big|_{z=L} = 0$ and with the initial condition $V\big|_{t=0} = \varphi(z)$, we are using the explicit difference scheme (DS) with the second order of approximation:

$$\begin{cases} V_i^{m+1} = V_i^m + th / \mu\left(V_{i-1}^m - 2V_i^m + V_{i+1}^m\right) - \tau g_i^m \\ V_0^m = \tilde{V}_0, V_{N+2}^m = V_N^m, V_i^0 = \varphi(z_i),\ i = \overline{2, N1},\ m = \overline{1, M} \end{cases}, \qquad (4.1)$$

where V_i^m is the approximated value of the $V(z_i, t_m)$, $z_i = (i-1)h$, $Nh = L$, $t_m = m\tau$, $N1 = N + 1$, h, τ are the corresponding steps of space and time, N, M are the number of the above - mentioned steps, $th = \tau / h^2$. The (DS)'s (4.1) stability condition is [2]: $\tau = h^2 \mu k_0 / 2$, $k_0 < 1$ (further as usually $k_0 = 1/2$). The (DS)'s (4.1) data processing with corresponding φ and $\tilde{V}_0$ is performed by MATLAB. Taking into account the values of V_1 and V_2, it is possible to calculate the values of temperature T and concentration of moisture C in the grid points of (DS) using connections (3.3) and (3.4).

5. Numerical Solution in the Finite Layer by Solving the System of PDE for (T, C)

Applying the grid method, it is possible to solve directly both of them partial differential equations of the system (1.4) in the matrix – in vector form

$\partial W / \partial t = \tilde{M}_1 \partial^2 W / \partial z^2$, $W\big|_{z=0} = \tilde{W}_0$, $\partial W / \partial z\big|_{Z=L} = 0$, $W\big|_{t=0} = \phi(z)$, where $\tilde{M}_1 = \dfrac{1}{1-\lambda\nu}\begin{pmatrix} D^T & \nu D^C \\ \lambda D^T & D^C \end{pmatrix}$ - the second order matrix, $W = (T \quad C)^T$, $\tilde{W}_0 = (T_0 \quad C_0)^T$, $\phi = (\phi_1 \quad \phi_2)^T$ - vectors – columns. Then the vectors – difference equations (4.1) are in the form

$$V_i^{m+1} = W_i^m + th \cdot \tilde{M}_1 \left(W_{i-1}^m - 2W_i^m + W_{i+1}^m\right), i = \overline{2, N1}, \tag{5.1}$$

where W_i^m is the approximated value of $W(z_i, t_m)$, $W_0^m = \tilde{W}_0$, $W_{N+2}^m = W_N^m$, $W_i^0 = \phi(z_i)$.
In the moisturising problem $T_0 = 0$, $C_0 = 1$, $\phi_1 = \phi_2 = 0$, and in the drying problem $T_0 = 1$, $C_0 = 0$, $\phi_1 = 0$, $\phi_2 = 1$.
The stability condition of (DS) (4.1) is in the form

$$\tau \le \left(h^2 \left\|\tilde{M}_1\right\|^{-1} k_0\right) / 2 \tag{5.2}$$

If the present boundary conditions are not of the 1-th type, then the only possible way is numerical modelling of the initial system of (PDE) (1.3).
If the following conditions in the moisturising process are carried out $C\big|_{t=0} = T\big|_{t=0} = 0$, $C\big|_{z=0} = 1$, $(\partial T / \partial z)\big|_{z=0} = 0$ (the external temperature is not fixed), then for (DS) the approximation of the 1st equation of (PDE) (1.3) for grid point $z = 0\ (i = 1)$ in the form $T_1^{m+1} = T_1^m + 2th \cdot D^T \left(T_2^m - T_1^m\right)$ has to be solved additionally. The stability condition for these (DS) is in the form $\tau \le h^2 k_0 / \left(2D^T\right)$, and it is valid according to the condition (5.2) $\left\|\tilde{M}_1\right\| > D^T$.

6. The Evaluation of Numerical Results

Applying the mathematical system MATLAB, the numerical results for the moisturising and drying processes have obtained, $f_1 = f_2 = 0$, $D^C = 10^{-4}$, $D^T = 10^{-3}$, $L = 1/2$, $M = 50000$, $N = 50$, $h = 1/100$, if $\lambda\nu = 0.9$, then $\mu_1 = \mu_2$, (see appendix Table 1., 2., and Figure 1., 2.: the thickness of the material is marked off on the horizontal axis, but moisture concentration and temperature of material in dimensionless values in the fixed time moment on the vertical axis). The moisturising process is characterized by the increase in moisture concentration $C_{\inf}$ and C at constant temperature (Tab. 1. 1st row, Fig. 1., 2. on the left side, $C_{\inf}$, $T_{\inf}$ - values in the infinite media, C, T - values in the finite media). As the values of parameter λ decrease and the values of parameter ν increase, alongside with the increase in moisture concentration due to the absorption of water vapour, the increase in the temperature in the

interior part of material was observed (Tab. 1. 1. - 4. row), besides it is more characteristic for lesser λ and greater ν values. Rapid increase of temperature is more characteristic exclusively during the initial phase of the moisturising process, after prolonged time the temperature increase transfers to the more distant layers of material. Contrary to the moisturising process analysed above, the drying process with lesser λ values and greater ν values proceeds traditionally – the time t is characterised by the increase of temperature and decrease of moisture concentration in the internal part of material (Tab. 1. 5., 6. row, Fig. 1., 2. on the right side). On the contrary, with increasing the λ and with decreasing ν values alongside with the increasing the temperature in the internal part of material, there was observed also the increasing of moisture concentration in the border of the material. It is especially specific in the beginning of the drying process. Figure 2. allows comparing the moisturising and drying processes in the thick (theoretically – infinite) and in finite domain.
In the moisturising process the increasing of the moisture concentration more intensive occurs in the finite domain (Tab. 2., 1-th row - $C > C_{\inf}$). In the drying process both decreasing of the moisture concentration (Tab. 2., 2-th row - $C_{\inf} > C$) and increasing of the temperature (Tab. 2., 2-th row - $T > T_{\inf}$) intensive occurs in the finite domain.

6. Conclusions

The article contains numerical modelling of the system of two partial differential equations, which describes the distribution of temperature T and moisture C in porous medium depending on the physical parameters.

The obtained results can be used for:
1) Investigating dynamics of the moisture concentration and temperature change in time during the process of moisturising and drying of various porous materials as the process investigation is often related to technical difficulties and the process change dynamics can not be always characterised by measurements (for instance, high temperatures, continued process in time, etc.); 2) For modelling various porous materials depending on their characteristics and thus creating new materials with the desirable characteristics; 3) For investigating the increase of temperature during the moisturising process; 4) For investigating the effect of increase in moisture concentration during the drying process; 5) For investigating the effect of the increase in temperature and moisture concentration in relation to the physical and chemical parameters of the material under research.

References

[1] Crank, J.: *The mathematics of diffusion*. Oxford, Clarendon Press, 1956.
[2] Kalis, H.: *Skaitliskās metodes ar datorprogrammu MAPLE, MATHEMATICA lietošanu.* Rīga, LU, 2001.
[3] Morton K. W.: *Numerical solution of convection – diffusion problems*. Oxford, UK, Chapman & Hall, London, Inc., 1996.
[4] Тихонов, А., Самарский, А.: *Уравнения математической физики*. Москва, «Наука», 1966.

Authors

Dr.- Math., prof. Kalis, Harijs
Institute of Mathematics
Latvian Academy of Sciences and University of Latvia
Akadēmijas laukums 1
LV – 1524, Rīga, Latvija
E-mail: kalis@lanet.lv

Mg.- Math. Kangro, Ilmārs
Rēzekne Higher Educational Institution,
Department of Engineering Science
Atbrīvošanas aleja 90
LV – 4601, Rēzekne, Latvija
E-mail: kangro@ru.lv

Appendix

Tab. 1. Moisturising and drying parameter values and numerical results in a thick layer if z = 5

Parameters	λ	ν	t	T_{inf}	C_{inf}
1. Moisturising (Fig. 1)	9.0	0.1	50000	0.0059	0.0537
2. Moisturising	1.0	0.9	50000	0.0532	0.0537
3. Moisturising	3.0	0.3	50000	0.0177	0.0537
4. Moisturising	0.1	9.0	50000	0.5316	0.0537
5. Drying	0.1	9.0	50000	0.0537	1.0054
6. Drying (Fig. 1)	0.1	9.0	500000	0.1708	0.9010

Tab. 2. Moisturising and drying parameter values and numerical results in an infinite and finite layer if z = 0.5

Parameters	λ	ν	t	T_{inf}	C_{inf}	T	C
1. Moisturising	0.5	1.0	593.8	0.0612	0.1688	0.00723	0.3112
2. Drying	0.5	0.1	1181	0.7442	0.9418	0.9932	0.6163

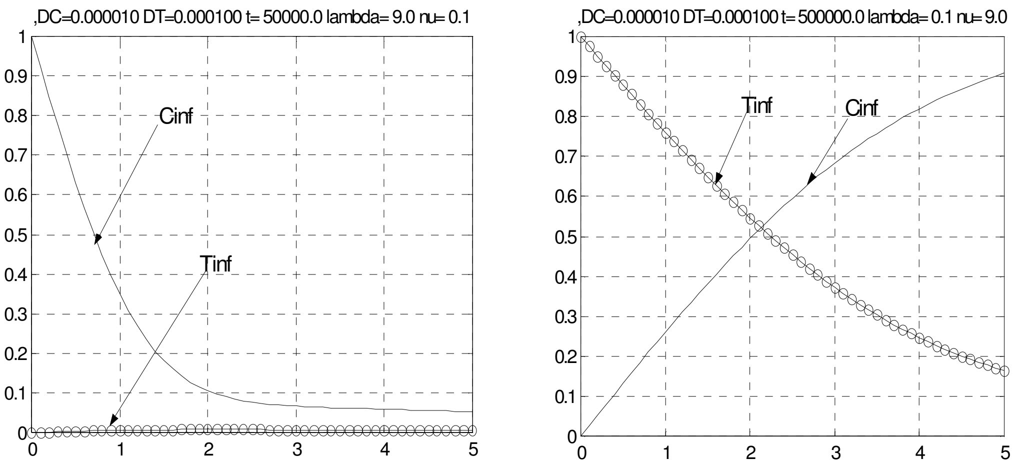

Fig. 1. Dependence of temperature and moisture concentration on parameters and during the moisturising (left side) and drying (right side) process in a thick domain

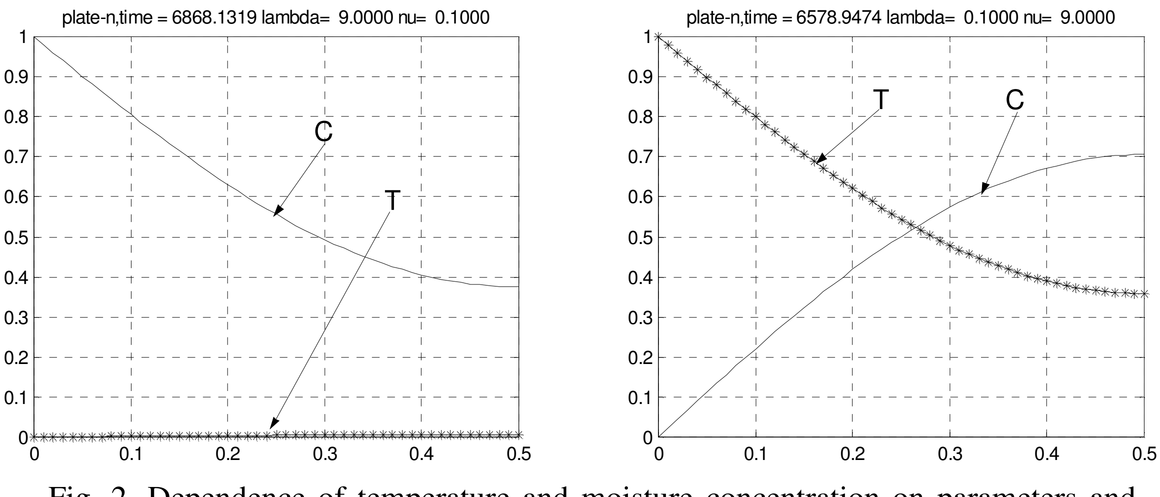

Fig. 2. Dependence of temperature and moisture concentration on parameters and during the moisturising (left side) and drying (right side) process in a finite domain